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SOP for Multiple Formulations and Preparations Regions of Responsibility Derived Using Dual-Energy CT


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|  Lawrence Livermore National Laboratory Global Security Principal Directorate Image Database Development Project | Standard Operating Procedure | |
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| SOP for Multiple Formulations and Preparations Regions of Responsibility Derived Using Dual-Energy CT | | |
| Concurrence <div style="text-align: right;">Technical Leader</div> | Date | |
| Approval <div style="text-align: right;">IDD Project Principal Investigator</div> | Date | |

1.0 Introduction

- 1.1 The purpose of this SOP is to specify the procedure used to aggregate Regions of Responsibility (RORs) from multiple formulations and preparations, each of which has its own ROR.
- 1.2 This SOP describes the procedure used to combine RORs for at least two formulations and preparations, each having been generated following the appropriate ROR generation SOP [SOP]. The RORs are two dimensional and have been constructed in the same feature space. The limits specified for the aggregate ROR are constructed by taking the convex hull [Wikipedia Page] of the corner points of the individual RORs. The convex hull of a set of two dimensional points can be visualized as the shape a rubber band would take if it were stretched around the outside of the points.

2.0 References

- 2.1 [SOP] Jeffrey S. Kallman, "SOP for Generation of Regions of Responsibility Using Dual-Energy CT", 2013.
- 2.2 [Wikipedia Page] http://en.wikipedia.org/wiki/Convex_hull
- 2.3 [Wikipedia Page 2] http://en.wikipedia.org/wiki/Convex_hull_algorithms

3.0 Definitions

| | |
|---------------|--|
| CT | Computed Tomography. A process by which the X-ray attenuation feature of a formulation and preparation may be measured. This may be performed at a single energy or multiple energies. |
| Feature | A measurable property of a formulation and preparation. While this should be a property that is measurable using X-ray CT (e.g. attenuation, Z_{eff} , Ratio of $\mu_{\text{low}}/\mu_{\text{high}}$), it could also be, e.g., bulk physical density, color, or taste. |
| Feature Space | A potentially multi-dimensional space in which the ROR is defined. The limits of the ROR for each dimension are computed and specified independently of all other dimensions. |
| Formulation | The process of physically mixing chemicals (i.e., without any significant chemical reactions occurring between them) to make an HME. Although chemical reactions may eventually occur between the component materials as the mixture ages, formulation does not rely on those effects to create the desired HME. Examples of formulations include blending two different solid powders (e.g., potassium chlorate and sugar), dissolving a solid in a liquid (e.g., sugar in hydrogen peroxide), binding a solid powder with a gel-like material (e.g., potassium chlorate and petroleum jelly), etc. |

| | |
|-------------|--|
| PI | Principal Investigator or responsible individual |
| Preparation | Method used to prepare a formulation for scanning |
| ROR | Region of Responsibility. This defines the portion of the specified feature space in which the vendor is responsible for finding the particular explosive formulation and preparation. |
| SOP | Standard Operating Procedure. |

4.0 Roles, Responsibilities and Authority

4.1 Roles:

- 4.1.1 LLNL: Honest Broker, X-ray Physics SME
- 4.1.2 TAFL: HME data collection synthesis lab
- 4.1.3 TSL: Conventional and Military data collection synthesis lab
- 4.1.4 TSA/OSC: End user of data collected under this program
- 4.1.5 EXD: Technical oversight and data collection process manager

4.2 The HME Working Group has the overall responsibility and authority for this procedure.

4.3 Original Standard Operation Procedures shall have the signature form completed prior to the effective date.

4.4 Laboratories (e.g. LLNL, TAFRL and TSL) using this SOP to aggregate RORs are responsible for assuring the quality of the data used and checking the formulation and preparation RORs before using the resultant aggregate ROR.

5.0 Safety

6.0 Procedure

- 6.1 Collect the points that define the perimeter of each individual formulation and preparation ROR into a single table.
- 6.2 Use any of the available convex hull algorithms [Wikipedia Page 2] to determine the convex hull of the aggregate ROR space.
- 6.3 Create a plot showing the limits of the aggregate ROR, the locations of the contributing individual RORs and the data points that were used to derive them. The X and Y axes will be determined by the features used in the study. Each formulation and preparation that was used should have a different symbol on the plot. The individual ROR limits should be plotted as a box enclosing the ROR. The aggregate ROR should be plotted as a polygon. Two examples are given in Appendix A.
- 6.4 Save the resulting tables and plots and record the results. Give these to the PI.

7.0 Document Revision History

| Date | Revision | Author | Responsible Manager | Comments |
|-----------|----------|--------------------|---------------------|---------------|
| 2/24/2014 | Rev #0 | Jeffrey S. Kallman | Harry E. Martz, Jr. | Initial draft |

Appendix A: Examples

Example 1: Generating an Aggregate ROR for Three Packings of As Received Tartaric Acid

Consider generating an aggregate ROR in $(\mu_{high}, {}^{LW}Z_{eff})$ space using RORs for each of three preparations of as-received Tartaric Acid scanned at LLNL.

Section 6.1: Collect the points that define the perimeter of each individual formulation and preparation ROR into a single table.

| | Pour ROR | | Tap ROR | | Tamp ROR | |
|--------------------|--------------|------------------|--------------|------------------|--------------|------------------|
| | μ_{high} | ${}^{LW}Z_{eff}$ | μ_{high} | ${}^{LW}Z_{eff}$ | μ_{high} | ${}^{LW}Z_{eff}$ |
| Lower Left | 656 | 7.341 | 699 | 7.265 | 817 | 7.205 |
| Lower Right | 826 | 7.341 | 940 | 7.265 | 972 | 7.205 |
| Upper Right | 826 | 7.395 | 940 | 7.462 | 972 | 7.585 |
| Upper Left | 656 | 7.395 | 699 | 7.462 | 817 | 7.585 |

Section 6.2: Use any of the available convex hull algorithms [Wikipedia Page 2] to determine the convex hull of the aggregate ROR space.

| Convex Hull of Pour, Tap, and Tamp RORs | |
|---|------------------|
| μ_{high} | ${}^{LW}Z_{eff}$ |
| 656 | 7.341 |
| 699 | 7.265 |
| 817 | 7.205 |
| 972 | 7.205 |
| 972 | 7.585 |
| 817 | 7.585 |
| 699 | 7.462 |
| 656 | 7.395 |

Section 6.3: Create a plot showing the limits of the aggregate ROR, the locations of the contributing individual RORs and the data points that were used to derive them. The X and Y axes will be determined by the features used in the study. Each formulation and preparation that was used should have a different symbol on the plot. The individual ROR limits should be plotted as a box enclosing the ROR. The aggregate ROR should be plotted as a polygon. Figure A-1 shows this plot for this example. Figure A-2 shows just the aggregate ROR.

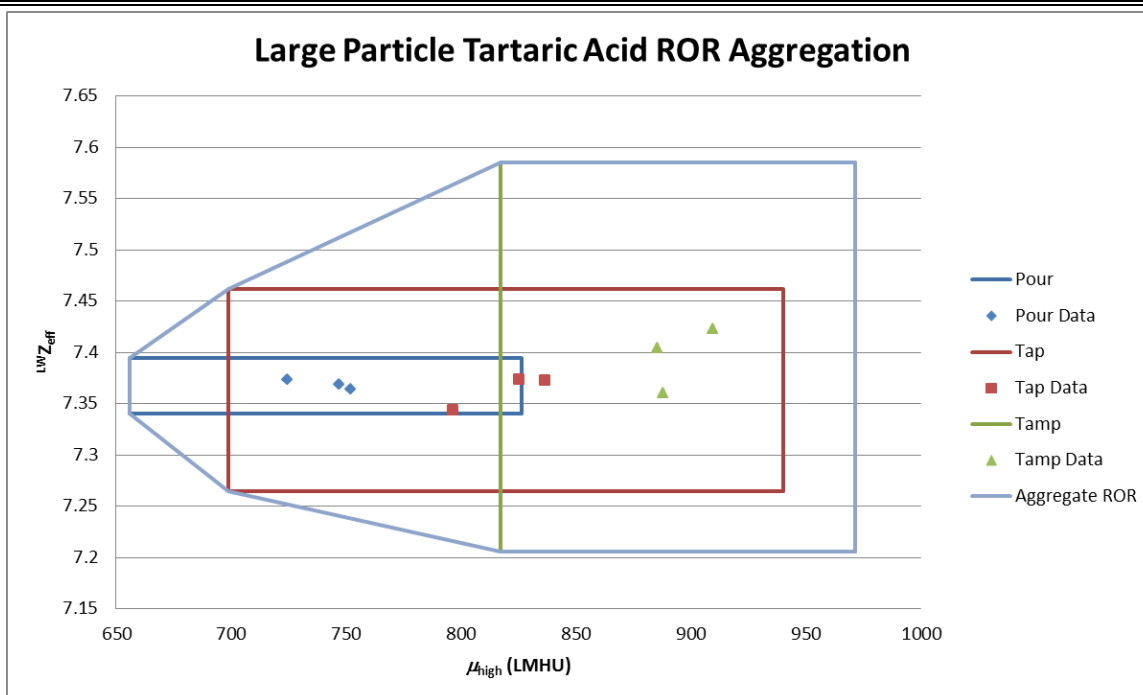


Figure A-1. This plot verifies that the convex hull is correctly aligned to the individual formulation and preparation RORs.

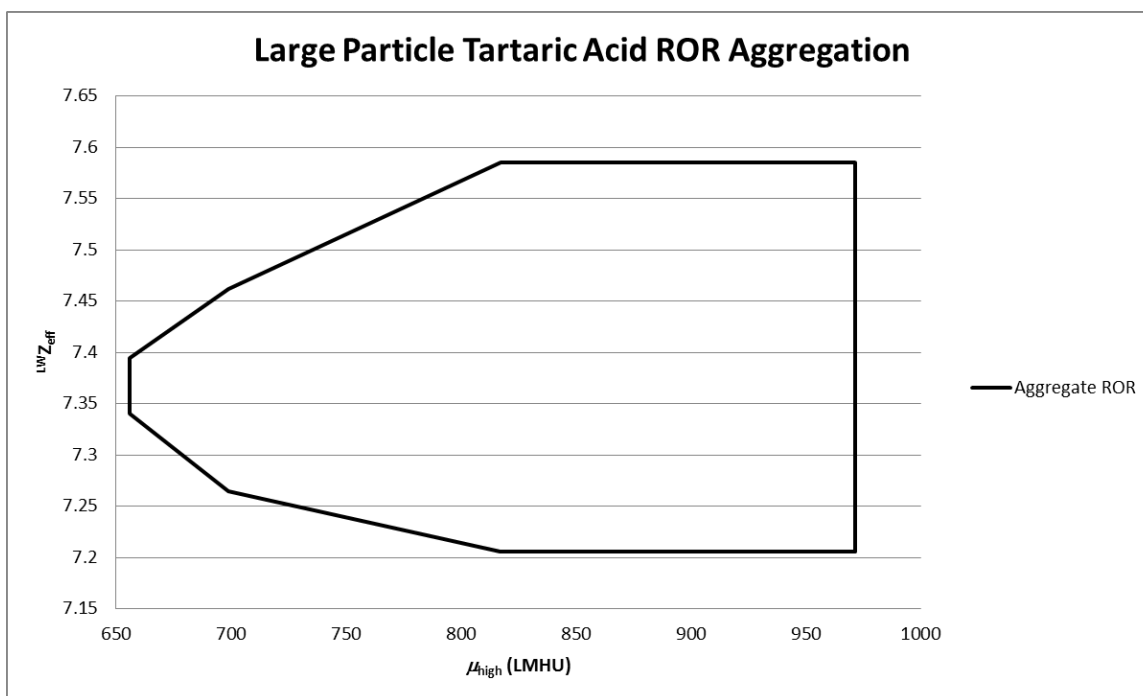


Figure A-2. This plot shows the aggregate ROR for as-received Tartaric Acid for three preparations.

Example 2: Generating an Aggregate ROR for Four Fictitious Formulations and Preparations

Consider generating an aggregate ROR in (Feature1, Feature2) space using RORS for each of four fictitious formulations and preparations.

Section 6.1: Collect the points that define the perimeter of each individual formulation and preparation ROR into a single table.

| | F&P 1 | | F&P 2 | | F&P 3 | | F&P 4 | |
|--------------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| | Feature 1 | Feature 2 | Feature 1 | Feature 2 | Feature 1 | Feature 2 | Feature 1 | Feature 2 |
| Lower Left | 79 | 1.20 | 139 | 0.74 | 35 | 2.60 | 162 | 1.96 |
| Lower Right | 113 | 1.20 | 159 | 0.74 | 123 | 2.60 | 193 | 1.96 |
| Upper Right | 113 | 1.77 | 159 | 2.51 | 123 | 3.28 | 193 | 3.01 |
| Upper Left | 79 | 1.77 | 139 | 2.51 | 35 | 3.28 | 162 | 3.01 |

Section 6.2: Use any of the available convex hull algorithms [Wikipedia Page 2] to determine the convex hull of the aggregate ROR space.

| Convex Hull of 4 F&P RORs | |
|---------------------------|-----------|
| Feature 1 | Feature 2 |
| 139 | 0.74 |
| 159 | 0.74 |
| 193 | 1.96 |
| 193 | 3.01 |
| 123 | 3.28 |
| 35 | 3.28 |
| 35 | 2.60 |
| 79 | 1.20 |
| 139 | 0.74 |

Section 6.3: Create a plot showing the limits of the aggregate ROR, the locations of the contributing individual RORs and the data points that were used to derive them. The X and Y axes will be determined by the features used in the study. Each formulation and preparation that was used should have a different symbol on the plot. The individual ROR limits should be plotted as a box enclosing the ROR. The aggregate ROR should be plotted as a polygon. Figure A-3 shows this plot for this example. Figure A-4 shows just the aggregate ROR.

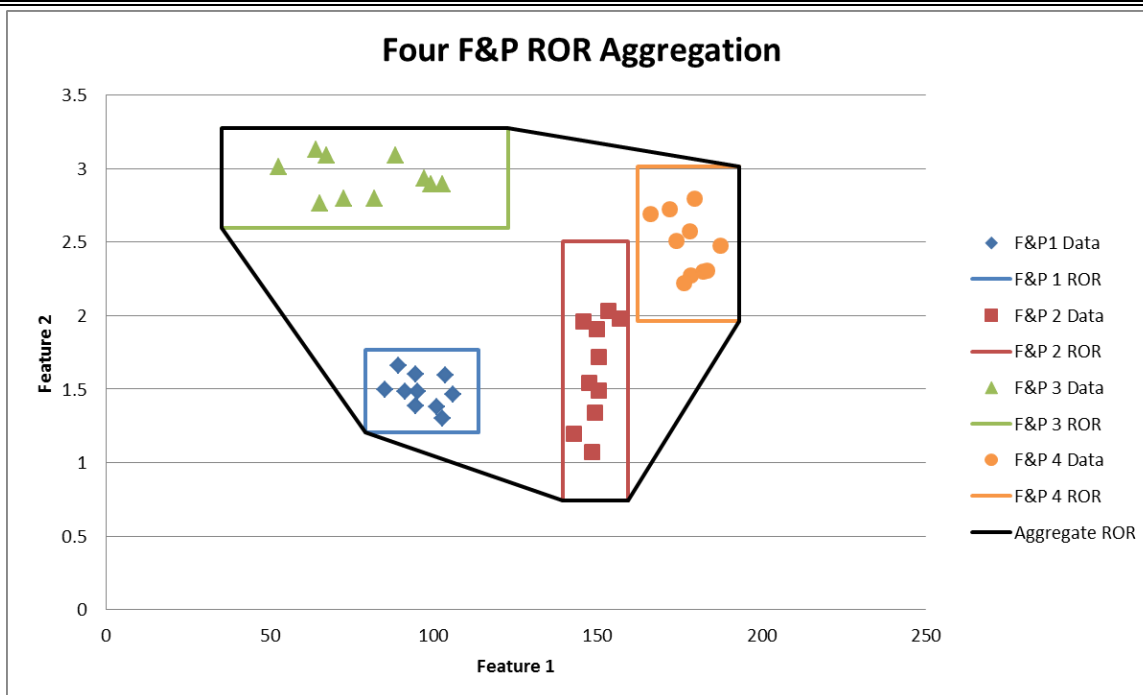


Figure A-3. This plot verifies that the convex hull is correctly aligned to the individual formulation and preparation RORs.

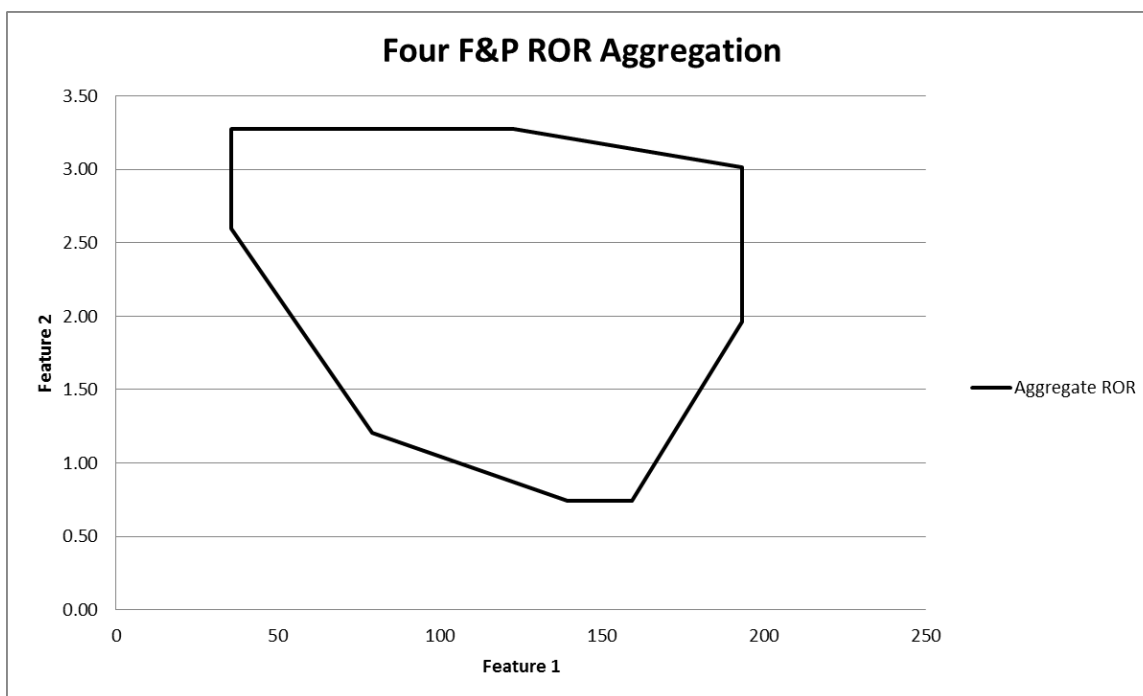


Figure A-4. This plot shows the aggregate ROR for the four formulations and preparations.